



chain nodes :

21 22 23 24 25 26 27 28 29 30 31 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

4-25 12-26 14-27 15-17 17-28 18-21 18-31 19-22 19-30 20-23 20-29 23-24 25-26

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-13 6-15 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15
16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

4-25 5-13 6-15 13-14 14-15 15-17 16-17 16-20 17-18 18-19 18-21 19-20 19-22

exact bonds :

12-26 14-27 17-28 18-31 19-30 20-23 20-29 23-24 25-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:Atom